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14. ABSTRACT
The general aim of the proposed research is to understand how nanoscale laminates with optimal strength, ductility, and elevated temperature stability can be engineered through the selection of component chemistry, component layer thickness, and interfacial and grain boundary structure. The first effort is to develop computational tools to model the deformation and fracture processes in nanoscale laminates based on a well-known intermetallic system. The second effort is to apply the computational tools to at least one additional laminate system.

This report describes our efforts over the past year to model critical features which control the strength of interfaces to dislocation transmission, and to study the morphological stability of Ni(Al)/Ni3Al that are heated to elevated temperature for prolonged periods. These two areas are critical to optimizing both the plastic strength and elevated temperature stability of nanoscale materials.

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MULTILAYERED MATERIALS, NANOLAMINATED COMPOSITES, STRENGTH, MAGNETRON SPUTTERING, FRACTURE, DISLOCATION TRANSMISSION, INTERFACIAL STRENGTH.

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Final Technical Report

1 JAN 00 to 31 MAR 01

DEFORMATION MECHANISMS IN MULTILAYERED MATERIALS FOR HIGH TEMPERATURE APPLICATION

GRANT NUMBER: F49620-00-1-0089

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Abstract

The aim of the proposed research is to understand how nanoscale laminates with optimal strength, ductility, and elevated temperature stability can be engineered through the selection of component chemistry, component layer thickness, and interfacial and grain boundary structure. The first effort is to develop computational tools to model the deformation and fracture processes in nanoscale laminates based on a well-known intermetallic system. The second effort is to apply the computational tools to at least one additional laminate system.

Research Objectives

Develop computational tools based on the observed physical phenomena of dislocation motion and fracture, so that strength can be predicted as a function of layer thickness, interfacial structure, and crystal orientation.

Summary of Research Findings and Activities

Transmission of Slip and Cracks Across Interfaces

Ultimately, multilayer samples fail by the propagation of slip and or cracks across interfaces, so that the cross section under tension fails by a combination of plastic necking or fracture. Figure 1 shows a side view of a 120nm/120nm γ-Ni(Al)/γ'-Ni_3Al multilayer that was pulled to failure in tension. The noticeable plastic deformation is evidence of the large amount of slip propagation across interfaces that can accompany failure.

A dislocation analysis indicates that the critical resolved shear stress for the leading dislocation in a pile-up to transmit across the interface can be approximated by

$$\frac{\tau_{transmit}(N)}{\mu'} \approx \frac{N}{2\pi h / b} + \frac{\boxed{\tau^*_{int}}}{N\mu'} \qquad \tau^*_{int} \approx \tau^*_{coh} + \frac{2e(h,s)}{bs}$$

where $\mu' = \mu/(1 - \nu)$ is a function of the effective elastic shear modulus μ and Poisson's ratio ν and $\tau_{int}{}^*$ is the strength of the interface to slip transmission, expressed as the critical resolved shear stress to push a dislocation across the interface. The relation also shows that the strength of the interface consists of the value, $\tau_{coh}{}^*$, for a coherent interface, plus the additional strength associated with pinning by misfit dislocations with spacing s. Our modeling with P.M. Hazzledine at UES, Inc. suggests that γ-Ni(Al)/γ'-Ni_3Al multilayers have a larger $\tau_{int}{}^*$ at larger h, when interfaces are

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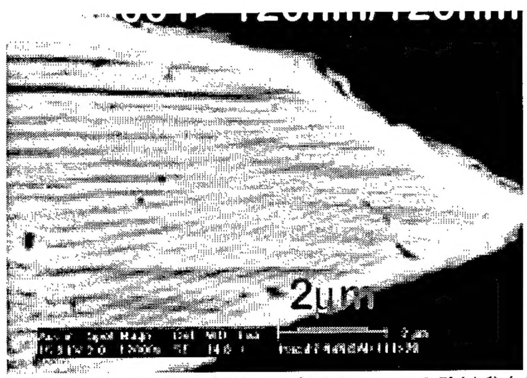

Figure 1: SEM image of a side view of a 120nm/120nm γ-Ni(Al)/γ'-Ni_3Al multilayer that was pulled to failure in tension.

semi-coherent, and have a smaller τ_{int}^* at smaller h (< 50nm), when interfaces are coherent. In fact, we have substituted into the above equation the dislocation theory solution for the equilibrium value of s as a function of h.

When $\underline{\tau_{transmit}}$ (N) and $\underline{\tau_{CLS}}$ (N) are equated, the result is that multilayers have a critical layer thickness at which the critical resolved shear stress for pile-up transmission is largest.

Figure 2 shows that there is a multilayer design curve relating the strength of interfaces to the layer thickness. For stronger interfaces and/or large layer thickness, the multilayer is predicted to deform by confined layer slip, with subsequent pile-up and ultimately dislocation transmission. Multilayer strength in this regime is expected to increase with decreasing layer thickness. For weaker interfaces and/or smaller layer thickness, the multilayer is predicted to deform first by dislocation transmission across interfaces and then multiple layer slip. In this regime, decreasing layer thickness is not expected to significantly increase multilayer strength.

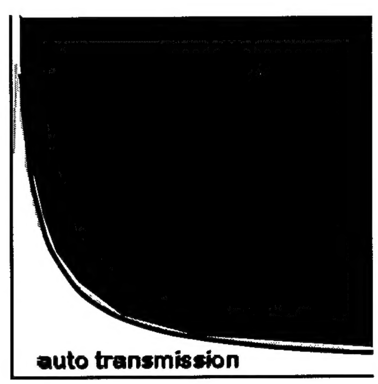

Figure 2: A plot of interfacial strength to slip transmission versus individual layer thickness for multilayers, showing two distinct plasticity regimes.

Our focus effort over the past year has been to understand how τ_{coh}^* depends on the properties of the A and B phases and the interface between them. This work is motivated by our observation that the room temperature plastic strength of multilayers may be increased by increasing the resistance of interfaces to slip transmission. A simple model is considered in which a screw dislocation lies parallel to an interface and glides along a slip plane that is perpendicular to the interface. A Peierls model of the dislocation is used, and the evolution of the dislocation core is studied during dislocation transmission across the interface. A significant finding is that the strength of the interface to transmission can be increased by making the easier to slide. This is accomplished by decreasing the unstable stacking fault energy of the interface. Figure 3 shows the critical core configurations during transmission of a screw dislocation across interfaces that have a larger (Figure 3a) versus smaller (Figure 3b) unstable stacking fault energy, assuming an elastic modulus mismatch of 10%. The interfacial sliding traps the core and produces an interfacial strength that is more than three times the interfacial strength for a nonsliding interface (Figure 3a). Current efforts are to simulate the transmission of a dislocation from the disordered γ-Ni(Al) phase into the ordered γ'-Ni_3Al phase.

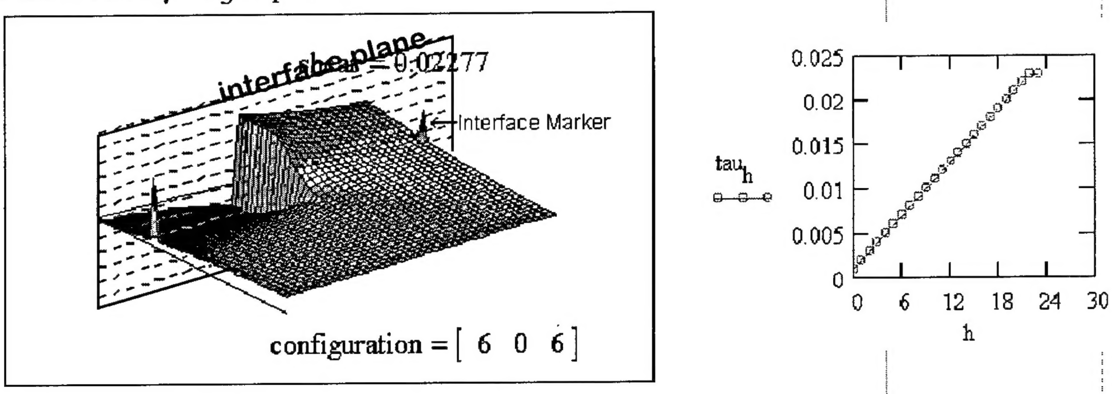

Figure 3(a): Critical core configuration for a screw dislocation as it transmits across interface into a material with an elastic modulus that is 10% larger, based on a Peierls model analsis. The unstable stacking fault energy assigned to the interface is large enough so that the interface does not slide.

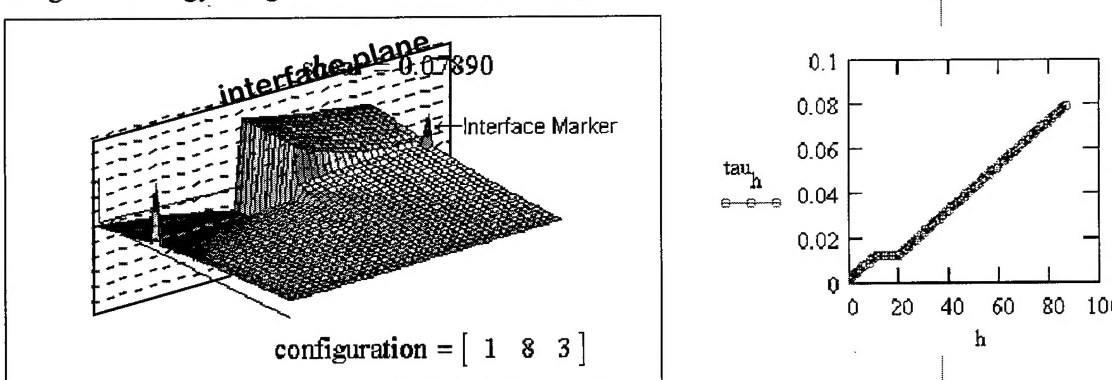

Figure 3(b): Critical core configuration for a screw dislocation as it transmits across interface into a material with an elastic modulus that is 10% larger, based on a Peierls model analsis. The unstable stacking fault energy assigned to the interface is 60% of that used to produce Figure 3a. The spreading of the dislocation core into the interface produces significant trapping of the dislocation in the interface.

Morphological Stability of γ-Ni(Al)/γ'-Ni_3Al Multilayers at Elevated Temperature

Near the end of this award period, we began heating γ-Ni(Al)/γ'-Ni_3Al multilayers to various temperatures and times to study the morphological stability at elevated temperature. Figure 4(a,b) show SEM micrographs of 120nm/120nm [001] texture samples after heating for 20 hours at 800C and 1100C, respectively. At 800C, there is noticeable evidence of morphological breakdown, in the form of γ'-Ni_3Al layers which have pinched off. At 1100C, complete breakdown has occurred and a particulate morphology is produce, with cuboidal particle which appear to be oriented to the local [001] crystallographic direction in the surrounding γ-Ni(Al) phase. Current efforts are to study the effect of precipitates, stress, and crystallographic texture on the stability of this system.

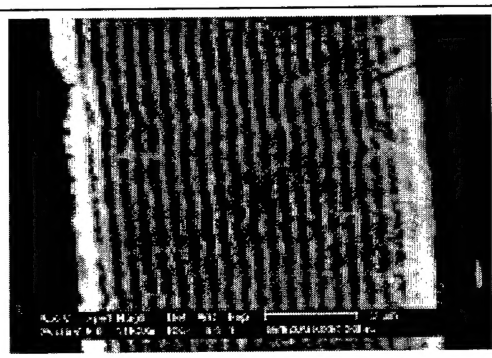

Figure 4(a): SEM micrograph of a γ-Ni(Al), Ni_3Al 120nm/120nm multilayer after expos to 800C for 20hrs in Argon, followed by cool to room temperature.

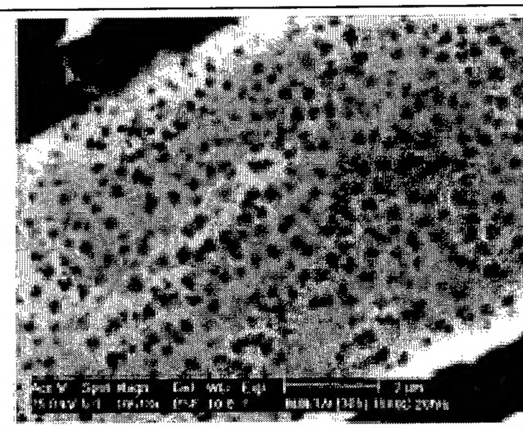

Figure 4(b): SEM micrograph of a γ-Ni(Al) Ni_3Al 120nm/120nm multilayer after expos to 1100C for 20hrs in Argon, followed cooling to room temperature.

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Publications

"A Peierls Approach to the Critical Shear Stress for Dislocation Transmission Through a Bi-material Interface", Anderson, P.M. and Xin, X., J.R. Rice 60th Anniversary Vol. (J. Chuang, ed.,) Kluwer Publishers, Dordrecht (2000).

"A Peierls Analysis of the Critical Stress for Transmission of a Screw Dislocation Across a Coherent, Sliding Interface,"Z. Li and P.M. Anderson, accepted for publication in *Mater. SciEng. A.*, Dec. 2000.

"Influence of Crystallographic Orientation and Layer Thickness on the Fracture Behavior of Ni/Ni3Al Multilayered Thin Films", R. Banerjee, J.P. Fain, P.M. Anderson, and H.L. Fraser, accepted for publication in *Scripta Mater.*, February, 20001.

Awards Received

Presented two invited presentations at the Fall 2000 MRS Meeting that were based on AFOSR funded work.

Transitions

none